

Supplemental Table S1. Data collection and refinement statistics

Data Set	BAKQ77L PDB: 5fmi	BCL-X _L :hBAKBH3 PDB: 5fmk	BCL-X _L :mBakBH3 Q75L PDB: 5fmj
Crystal Parameters			
Space group	C 1 2 1	C 1 2 1	P 6 ₁ 2 2
Unit Cell Parameters			
<i>a, b, c</i> (Å)	58.024, 54.528, 58.716	77.668, 55.459, 61.053	57.789, 57.789, 268.327
α, β, γ (°)	90, 115.5, 90	90, 127.12, 90	90, 90, 120
Data Collection			
R _{merge}	0.028 (0.158)	0.036 (0.301)	0.085 (0.757)
I/σ(I)	26.6 (7.5)	35.22 (4.73)	27.6 (3.8)
Completeness (%)	98.9 (99.6)	99.38 (95.42)	99.3 (98.3)
Redundancy	3.7 (3.7)	3.7 (3.5)	19.2 (14.9)
No. of copies/a.s.u.	1	1	1
Refinement			
Resolution (Å)	26.19-1.49 (1.54-1.49)	19.40-1.73 (1.81-1.73)	19.66-2.43 (2.67-2.43)
No. of reflections R _{work}	26752 (2544)	21521 (2488)	10808 (2438)
No. of reflections R _{free}	1388 (134)	1105 (110)	540 (129)
R _{work}	0.1855 (0.1816)	0.1575 (0.2062)	0.1799 (0.2239)
R _{free}	0.2115 (0.1983)	0.1856 (0.2230)	0.2195 (0.2915)
No. of atoms			
Protein	1316	1395	1446
Ligand	3	24	16
Solvent	131	123	40
R.M.S. Deviations			
Bond lengths (Å)	0.005	0.005	0.009
Bond angles (°)	0.705	0.723	0.935
Chiral (Å ³)	0.067	0.047	0.048